Mechanism for stabilization of a spin liquid in a Kondo lattice

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A mechanism is proposed for stabilization of a spin liquid of neutral fermions in a Kondo lattice. A single-site Kondo scattering of conduction electrons at temperatures T above the Kondo temperature T_K not only suppresses the antiferromagnetic order but also promotes the onset of an RVB state. The Kondo scattering "freezes" at $T^* > T_K$. In the limit $T \to 0$, the system thus behaves as a two-component Fermi liquid with neutral and charged components.

1. The unusual behavior of heavy-fermion systems stems from a transformation of the properties of the spins of the rare earth ions in these systems upon the transition from the "high-temperature" region $T > T^*$, where they behave as ordinary localized moments, to the low-temperature region $T < T_{\rm coh} \ll T^*$, where the entire thermodynamics is governed by Fermi branches of excitations. Since the number of spin degrees of freedom (~ 2 per unit cell) is considerably larger than the number of charge degrees of freedom which are involved in the formation of heavy fermions ($2T^*/\varepsilon_F$ per unit cell), it is natural to assume that these spin degrees of freedom constitute the source of the anomalously high density of fermion excitations at $T < T^*$.

In contrast with the conventional understanding (Refs. 1–3, for example), which relates the conduction electrons with f-wave spins in a state of "Kondo singlets," a scenario discussed in Refs. 4 and 5 has a two-component Fermi liquid with a neutral spin component and a charged electron component. In the present letter we propose a microscopic mechanism for the formation of a neutral spin liquid. We show that single-site Kondo scattering at high temperatures $T > T_K$ promotes stabilization of this liquid with respect to both antiferromagnetic ordering and the formation of a coherent Kondo-singlet state.

2. Heavy-fermion compounds with an integer valence are described by the effective sf-exchange Hamiltonian

$$H_{\rm eff} = \sum_{\mathbf{k}\sigma} \varepsilon_k c^+_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + J_{sf} \sum_{\mathbf{i}} \mathbf{s}_{\mathbf{i}} \cdot \mathbf{S}_{\mathbf{i}}. \tag{1}$$

Here ε_k are the energy levels of the conduction electrons in the band, whose width is characterized by the Fermi energy ε_F; the operators $\mathbf{S}_{\mathbf{i}}$ and $\mathbf{s}_{\mathbf{i}} = c^+_{\mathbf{i}\sigma} \hat{\sigma} c_{\mathbf{i}\sigma}$ represent localized f-wave spins and the spins of conduction electrons, respectively; and $\hat{\sigma}$ is the Pauli matrix. A regular perturbation theory for the Kondo lattice described by Hamiltonian (1) can be formulated only for high temperatures $T > T_K$, at which the approximation of

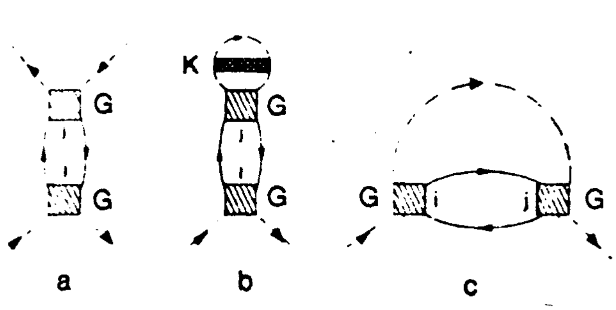

FIG. 1. Effective vertex (a) and eigenenergy parts of the pseudofermion Green's functions (b and c).

noncrossing diagrams[1] is valid. In that approximation, the Kondo scattering at each lattice site can be treated independently, and the scattering itself can be dealt with in the logarithmic approximation. According to Doniach,[6] this approximation leads to a competition between an antiferromagnetic state, which is realized at small values of the effective coupling constant $\alpha = J_{sf}/\varepsilon_F$, and a nonmagnetic Kondo-singlet state, which should form at large values of α. We see, however, that in the critical region $\alpha_{c0}^2 \approx \exp(-1/2\alpha_{c0})$, i.e., at $T_N \approx T_K$, where $T_{N,K}$ are the Néel and Kondo temperatures, respectively, a third possibility is realized: A spin liquid of the resonating-valence-bond (RVB) type[7] arises with a characteristic energy $T^* > T_K$. The Kondo scattering freezes at $T \sim T^*$, but the possibility of significant antiferromagnetic correlations persists.

We will use the standard technique of temperature Green's functions, introducing the representation of Abrikosov pseudofermions for the spin operators $\mathbf{S}_\mathbf{i} = f^+_{\mathbf{i}\alpha} \hat{\sigma}_{\alpha\beta} f_{\mathbf{i}\beta}$. At $T > T_K$, we use the approximation of noncrossing diagrams (NCA), in which single-site Kondo processes can be treated independently, without consideration of other sites. In this approximation, the intersite interaction is described by indirect RKKY exchange (see Fig. 1, where the solid and dashed lines represent electron and pseudofermion propagators, respectively). The effect of multiple Kondo scattering is seen in a renormalization of the single-site vertex parts. Their strengthening in the logarithmic approximation is known:[8] $\Gamma(\varepsilon) = J_{sf}\{1 - 2\alpha \ln[\varepsilon_F/\max(\varepsilon, T)]\}^{-1}$. In calculating the indirect intersite exchange, we consider only nearest neighbors in the polarization operator: $\Pi_\mathbf{q}(i\omega_n) = \Pi_R(i\omega_n) S^{(1)}(\mathbf{q})$, where $S^{(1)}(\mathbf{q}) = \Sigma_1 \exp i\mathbf{q}\cdot(\mathbf{j}-\mathbf{l})$ is a structure factor, and $R = |\mathbf{j}-\mathbf{l}|$. In this approximation, the Fourier component of the static RKKY interaction, $\tilde{J}(R,T) S^{(1)}(\mathbf{q})$, is expressed in terms of an effective constant:

$$\tilde{J}(R,T) = T \sum_n G^2(R, \varepsilon_n) \Gamma^2(\varepsilon_n, T), \tag{2}$$

where the electron Green's function is taken in the following asymptotic form[9] in the coordinate representation at imaginary frequencies:

$$G(R,\varepsilon) = -\frac{v_F}{2\pi p_F R} \exp\left(-\frac{|\varepsilon| R}{v_F} + i p_F R \,\mathrm{sgn}\,\varepsilon \right). \tag{3}$$

Substituting (3) into (2), we find

$$\tilde{J}(R,T)\approx\Phi(p_FR)\alpha^2\int_T^{\varepsilon_F}d\varepsilon\frac{\exp\left(-\frac{\varepsilon}{\varepsilon_F}p_FR\right)}{\left[1+2\alpha\ln\frac{\varepsilon}{\varepsilon_F}\right]^2}. \quad (4)$$

Here $\Phi(x)$ is an oscillating RKKY function. The energy dependence of the single-site vertex parts of $\Gamma(\varepsilon)$ leads to a sharp change in the temperature dependence of the RKKY interaction at $T\ll\varepsilon_F$. Instead of the factor $\exp[-(T/\varepsilon_F)p_FR]\approx 1$, which is essentially independent of the temperature, a logarithmic strengthening of the type $\ln^{-n}(T/T_K)$ arises near the Kondo temperature. Asymptotic estimates and numerical calculations from expression (4) show that the exponent here is $n\approx 1$.

In the pseudofermion Abrikosov representation, the interaction in the spin subsystem is thus described by an effective four-fermion vertex (Fig. 1a). Possible correlated states of this subsystem can be described by the mass operators shown in Fig. 1, b and c (cf. Ref. 2). The diagram in Fig. 1b, in which the pseudofermion lines are closed at one site, corresponds to a commensurate magnetic order with an antiferromagnetic vector $\mathbf{Q}$ satisfying $\mathbf{Q}\cdot\mathbf{R}_{ij}=\pi$. The order parameter of the antiferromagnetic phase is the Néel molecular field $B_N(T)=\lambda_1\tilde{J}(R,T)\langle S_z\rangle$, where the expectation value of the spin of a site is expressed in the standard way in terms of the expectation values of the pseudofermion operators: $\langle S_z\rangle=\langle f^+_{i\uparrow}f_{i\uparrow}-f^+_{i\downarrow}f_{i\downarrow}\rangle$ (the closed loop on the diagram in Fig. 1b). Here the numerical factor λ_1 is determined by the geometry of the lattice. In the NCA, Kondo processes lead to a temperature-dependent screening of the spin expectation value[10,8] $\langle S_z\rangle$ at each lattice site (K in Fig. 1b). The result of an exact solution of the single-site Kondo problem[8] is a function $K(T)$ which falls off monotonically with decreasing temperature and which has a finite value $[K(T_K)\approx 0.37]$ at the Kondo temperature. The self-consistent equation for the temperature of the transition to the antiferromagnetic state differs from the ordinary equation for the order parameter in that there is a screening correction $K(T)$:

$$\langle S_z(T_N)\rangle=\tfrac{1}{2}K(T_N)\tanh\frac{B_N(T_N)}{2T_N}. \quad (5)$$

Here T_N is defined as the temperature at which a nontrivial solution of the equation for $\langle S_z\rangle$ arises.

Resonating valence bonds are an alternative possibility for the onset of a correlated state of a spin subsystem, specifically, a spin-liquid state. In this phase, the spins of neighboring f-electrons are bound in pairs in singlet states, which are characterized in the mean-field approximation by a nonvanishing "order parameter" $\Delta_{\mathrm{RVB}}=\Sigma_\sigma\langle f^+_{i\sigma}f_{j\sigma}\rangle$ (see, for example, Refs. 2, 7, and 11). The difference between the "anomalous" expectation value and zero corresponds to closure of the pseudofermion lines of different sites in Fig. 1c. The order parameter defined in this manner describes a homogeneous spin liquid.

In the nearest-neighbor approximation, a Fermi spectrum of elementary excitations with a dispersion relation $u(k)\sim\Delta_{\mathrm{RVB}}\alpha^2\varepsilon_FS^{(1)}(\mathbf{k})$ corresponds to an RVB state. In general, the magnitude of the mean field is given by the expression $B_{\mathrm{RVB}}(T)=\Sigma_m\tilde{J}^{(m)}\times(R_m,T)\Delta^{(m)}_{\mathrm{RVB}}S^{(m)}(\mathbf{k})$, where the summation is over coordination spheres (m) for which

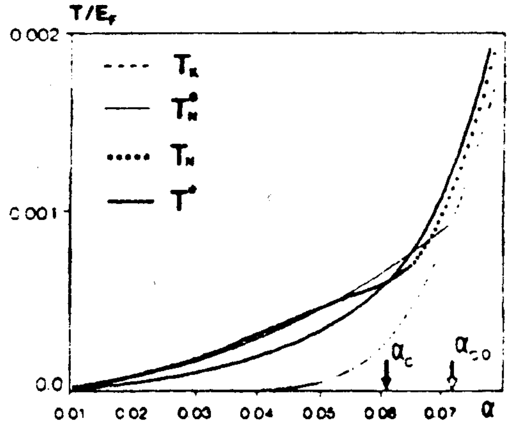

FIG. 2. Modified Doniach diagram for competing Néel and RVB phases for the parameter values $z=6$, $\lambda_1/\lambda_2=2.1$, and $p_F R=2.88$. Here α_{c0} and α_c are critical points, at which the antiferromagnetic solution disappears from the standard and modified Doniach diagrams.

the indirect exchange has an antiferromagnetic sign.[11] The diagram in Fig. 1c contributes a self-consistent equation for the temperature at which the system goes into the spin-liquid state:

$$\Delta_{\mathrm{RVB}}(T^*)=(zN)^{-1}\sum_{\mathbf{k}} S^{(1)}(\mathbf{k})\tanh\frac{B_{\mathrm{RVB}}(T^*)}{2T^*} \tag{6}$$

(cf. Refs. 2 and 11). Here T^* is defined as the temperature at which a nontrivial solution of the equation for Δ_{RVB} with $m=1$ and a coordination number z arises.

Using (2) and (4) to calculate the molecular fields $B_N(T)$ and $B_{\mathrm{RVB}}(T)$, we find

$$B_N(T)\simeq B_N^0(T)K(T)\ln^{-n}(T/T_K), \tag{7}$$

$$B_{\mathrm{RVB}}(T)\simeq B_{\mathrm{RVB}}^0(T)\ln^{-n}(T/T_K).$$

(The superscript 0 corresponds to the purely Heisenberg interaction J_{ij} without Kondo renormalizations.) Comparing these expressions, we see that the logarithmic intensification of the exchange due to Kondo scattering promotes the onset of both phases, but the screening of the spin $[K(T)]$ affects only T_N, weakening the tendency toward an antiferromagnetic pairing.

As a result, the Doniach phase diagram[6] (T_N^0, T_K versus α) is greatly modified in the critical region $\alpha\sim\alpha_c$, transforming into a diagram (T_N, T^* versus α) with a broad region in which the RVB phase exists. The shape of this diagram depends on the geometry of the lattice, the shape of the Fermi surface, and other factors. We have calculated the transition temperatures for spherical and cylindrical Fermi surfaces with RKKY functions $\Phi(x)\approx \pi x^{-3}\cos 2x$ and $\Phi(x)\approx -2x^{-2}\sin 2x$, respectively. We found that the region in which the RVB phase exists is wider in the latter case, which is close to the actual situation[12] in the heavy-fermion compound $CeRu_2Si_2$. Fig. 2 shows results calculated for a cylindrical Fermi surface. For the mean field B_{RVB} we used the approximation $B_{\mathrm{RVB}}(T)=\lambda_2\bar{J}^{(1)}(R,T)\Delta_{\mathrm{RVB}}^{(1)}S^{(1)}(\mathbf{k})$, where λ_2 is a geometric factor. In 3D Heisenberg lattices, the relation $\lambda_2<\lambda_1$ generally holds, and an RVB phase does not exist. However, Kondo scattering gives rise to a spin-liquid phase instead of a magnetic phase at $\alpha>\alpha_c$.

The critical region is characterized by the temperature hierarchy $T^* > T_N > T_K$. This result means that, first, the spins participating in RVB pairs are screened by the Kondo interaction to a substantial extent and, second, the neutral spin liquid is close to an antiferromagnetic instability. On the other hand, the Kondo scattering "freezes" at $T \approx T^* > T_K$, so single-site Kondo singlets do not form. The corresponding anomalous expectation values $\langle c_i^+ f_i \rangle$ introduced in the mean-field theories[2,3] with Hamiltonian (1) are actually zero. The Kondo temperature is no longer a singular point, and we can go to low temperatures, $T < T_K$, and take up the problem of a two-component Fermi liquid in which slow electrons with $\varepsilon < T_K$ interact with neutral spin fermions, whose spectrum is characterized by an energy T^*. The constant of this interaction can be estimated to be $\tilde{J}(T^*)$. This picture was proposed in Refs. 4 and 5 for describing the low-temperature properties of heavy-fermion systems (see also Refs. 13 and 14).

3. Many important effects remain outside the mean-field approximation. First, the "anomalous" expectation values $\Delta_{\rm RVB}$ are gauge-invariant. Incorporating fluctuations of the phase of the pseudofermions should lead to a conversion of the phase transition into a crossover. In the 2D $t-J$ model, incorporating uniform fluctuations of the gauge fields (chirality fluctuations) leads to an IR divergence.[15,16] In the 3D sf-exchange model, there is no such divergence. Furthermore, as can be seen from Fig. 2, the transition to the RVB phase occurs near an antiferromagnetic instability, so phase fluctuations are very nonuniform and have a spectral density of an antiparamagnon type. Incorporating retardation in the RKKY interaction in the diagram in Fig. 1b leads to a "polaron" renormalization $\sim \alpha^2 \omega \ln(\varepsilon_F/T)$ and to a damping $\sim \alpha^2 T$ of the spin fermions at T. The spin fermions themselves in turn have a strong influence on the low-frequency spectrum of electrons.[4,5,14,17] It can be assumed, however, that none of these phenomena substantially change the overall picture of the formation of a two-component Fermi liquid induced by Kondo scattering. According to this picture, Kondo processes in the lattice prevent the onset of an antiferromagnetic phase at parameter values in the critical region, $\alpha \sim \alpha_c$, while they simultaneously stabilize the spin-liquid state. The quantity T^* serves as a universal temperature which scales the properties of the heavy fermions. The heavy fermions themselves, however, become well-defined quasiparticles only at $T < T_{\rm coh} \ll T^*$, where their damping acquires a Fermi-liquid nature. In the crossover region, $T^* > T > T_{\rm coh}$, localized spins convert into neutral elementary excitations with Fermi statistics.

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